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OSTI-LLNL Scientific Analyses

Quality Implementing Procedure ID: OSTI-LLNL-QIP-SIII.5, Rev.0, Mod.0

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OSTI-LLNL
SCIENTIFIC ANALYSES

QA: QA

Quality Implementing Procedure ID: OSTI-LLNL-QIP-SIII.5, Rev.0, Mod.0 *Effective:* 2/25/05

1. PURPOSE

This Quality Implementing Procedure (QIP) establishes the responsibilities and the process for performing and documenting scientific and performance assessment analyses and calculations that are subject to the OSTI-LLNL Quality Assurance Plan (QAP) which implements the U.S. Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) Quality Assurance Requirements Description (QARD) DOE/RW-0333P. For the purposes of this procedure, scientific and performance assessment analyses and calculations are termed "analyses." This procedure may be used for analyses that are not subject to QAP requirements at the discretion of the Project Manager (PM). Planning requirements for conducting analyses are contained in OSTI-LLNL-QIP-2.2, *Planning for Science Activities.*

2. SCOPE

This QIP applies to the individuals within the Office of Science & Technology and International (OSTI)-Lawrence Livermore National Laboratory (LLNL) Project, and other participants who perform and document analyses in support of OSTI-LLNL activities. This QIP is prepared in accordance with OSTI-LLNL-QIP-5.0, *Preparing the Quality Assurance Plan and Quality/Technical Implement Procedures.*

3. PROCEDURE

3.1 PLANNING

The Technical Work Plan (TWP) must be completed before beginning action steps in Paragraph 3.1.1.

3.1.1 Project Manager (or designee):

A. Control the development, documentation, checking, change, and key technical activities of the scientific analysis activity in accordance with the requirements of this procedure. A Principal Investigator (PI) or Lead may be assigned to control these functions.

B. If a PI or Lead has been assigned, provide the PI/Lead with the applicable TWP prepared in accordance with OSTI-LLNL-QIP-2.2.

3.1.2 PI or Lead:

A. Review the TWP for the Work Package associated with the scientific analysis to be developed. If the TWP requires correction or revision,

ensure that it is completed in accordance with OSTI-LLNL-QIP-2.2 prior to continuing the analyses.

B. If a previously developed and validated model is to be used to conduct the scientific analysis, provide justification in the TWP that the present scientific analysis activity is within the intended use, limitations, and validity of the model.

C. Assign an Originator to perform the scientific analysis activity. (The Lead may assume the Originator's responsibilities; however, the Lead may not assume the Checker's responsibilities when acting as an Originator.)

3.2 DEVELOPMENT AND DOCUMENTATION OF ANALYSES

It is not necessary for the action steps to be performed sequentially.

3.2.1 Originator:

A. Perform the scientific analysis and associated tasks in accordance with the applicable TWP and all applicable procedures. Scientific notebooks may be used in the scientific analysis in accordance with OSTI-LLNL-QIP-SIII.0, *Scientific Notebooks.*

B. Obtain a document identifier (DI) for the scientific analysis from Document Control in accordance with OSTI-LLNL-QIP-6.0, *Controlled Documents.*

C. Document the scientific analysis in accordance with Attachment 1, Scientific Analysis Outline. If a section is non-applicable, indicate that it is non-applicable after the section title and provide a rationale for non-applicability.

D. If using a previously validated mathematical model to complete the scientific analysis, obtain the appropriate model file/product output from the OSTI-LLNL Technical Data Management System (TDMS).

E. If applicable, document technical product inputs used to develop the scientific analysis in the Document Input Reference System (DIRS) in accordance with BSC LP-3.15Q-BSC, *Managing Technical Product Inputs.*

F. Ensure the scientific analysis report is legible and in a form suitable for reproduction, filing, and retrieval.

G. Complete the appropriate portions of Attachment 2, Scientific Analysis Signature Page/Change History, in accordance with the instructions.

H. If qualified software is used in the analysis, ensure that it is controlled

and documented in accordance with OSTI-LLNL-QIP-SI.0, *Software Management.*

I. Document qualified software used in the scientific analysis in accordance with Section 3 of Attachment 1. Document that the use of the software was consistent with the intended use and within the documented validation range of the software.

J. Document the qualification of unqualified project data, developed in accordance with OSTI-LLNL-QIP-SIII.4, *Qualification of Unqualified Data,* in Section 6 of the Scientific Analysis Outline. The application of OSTI-LLNL-QIP-SIII.4 does not apply to Steps 3.2.1.K & L.

K. Data obtained from outside sources that are not established facts must be demonstrated to be suitable for the specific application. When appropriately justified, these data are considered qualified for use within the technical product. One or more of the following factors shall be used when presenting the case that data are suitable for intended use:

- Reliability of data source
- Qualifications of personnel or organizations generating the data
- Extent to which the data demonstrate the properties of interest
- Prior uses of the data
- Availability of corroborating data.

Note: External source data may still be qualified in accordance with OSTI-LLNL-QIP-SIII.4 (rather than suitable for intended use within the document text) when deemed appropriate.

L. Input obtained from the product output of a cancelled/superseded document must be demonstrated to be suitable for intended use and justified within the technical product. When appropriately justified, these inputs are considered qualified for intended use within the product. One or more of the following factors shall be used when presenting the case that inputs are suitable for intended use:

- .Reliability of input source.
- Qualifications of personnel or organizations generating the input.
- Extent to which the input demonstrates the properties of interest.
- Prior uses of the input.
- Availability of corroborating input.

Note: If the document and the product output have been superseded, the reason for supersession must be considered.

M. Software may be used prior to qualification to develop a preliminary output. Document and control the preliminary output in accordance with OSTI-LLNL-QIP-SIII.3, *Submittal and Incorporation of Data to the Technical Data Management System.* Reperform the work

producing the preliminary output to produce final output with baselined software in accordance with Paragraph 3.2.1.J) of this procedure. Make a comparison between the preliminary and final outputs. If the outputs are identical, then document the comparison and update the preliminary output with the final output on the Technical Data Information Form (from OSTI-LLNL-QIP-SIII.3). If the outputs are not identical, then document the comparison and supersede the Data Tracking Number (DTN) of the preliminary output with a new DTN containing the final output in accordance with OSTI-LLNL-QIP-SIII.3.

3.2.2 PI or Lead:

Ensure that the Originator has completed the appropriate steps as outlined in Paragraph 3.2.1.

3.3 CHECKING AND REVIEW

It is not necessary for the action steps to be performed sequentially. However, all action steps through Paragraph 3.3.6, with the exception of Paragraph 3.3.3.A.2), must be completed before beginning action steps in Paragraphs 3.3.7 through 3.3.12.

3.3.1 PI or Lead:

Assign a Checker to check the scientific analysis documentation. The Originator, Lead, or PI may not perform the checking function.

3.3.2 Originator:

Provide to the Checker and the Quality Assurance Representative (QAR) (an optional Scientific Analyses Checklist [Form 1097 on the BSC Intranet Automated Forms System] may be completed by the Originator):

1) Check copies of the scientific analysis documentation. Clearly indicate, on Attachment 2, one copy as the Checker Check Copy, and one copy as the QAR Check Copy, and initial and date.

2) The DIRS report, (if applicable).

3) Other supporting information and documentation that may be requested by the Checker or QAR.

3.3.3 Checker:

A. Check the scientific analysis documentation for the following (an optional Scientific Analyses Checklist [Form 1097 on the BSC Intranet Automated Forms System] may be completed by the Checker):

1) The content of the scientific analysis is technically adequate,

complete, and correct, and the documentation has been prepared in accordance with the requirements of this procedure and the applicable TWP.

2) Software, if used, is adequate for its intended use; is identified by software tracking number, title, and revision/version number; and has been controlled and documented in accordance with OSTI-LLNL-QIP-SI.0.

3) Appropriate product inputs were selected, identified in the documentation and on the DIRS report, and cited and incorporated in the scientific analysis activity, in accordance with BSC LP-3.15Q-BSC, when applicable.

4) TBV/Unresolved Reference Number tracking numbers, if any, are included in DIRS in accordance with BSC LP-3.15Q-BSC, when applicable.

5) The implications of uncertainties and restrictions are discussed and evaluated.

6) The assumptions, constraints, bounds, or limits on the inputs are identified in the documentation, and their impact on the results is described and assessed in the documentation.

7) The discussion of scientific approach and/or technical methods is documented.

8) The referencing is thorough, accurate, and complete, including appropriate project tracking numbers (e.g., records accession numbers, Technical Information Center numbers, DTNs), and is consistent with the DIRS report.

9) The appropriateness for using a previously developed and validated model to complete the present scientific analysis is described.

10) Data, information exchange drawings, and drawings used as direct inputs are verified to their home information system/controlled source (e.g., TDMS data are verified to TDMS DTNs via TDMS intranet).

11) All errata, initiated in accordance with OSTI-LLNL-QIP-16.0, *Condition Reporting and Resolution,* and documented against previous scientific analysis document revisions/changes, if any, are incorporated in the scientific analysis documentation.

12) The product output is accurate, correct, and technically adequate.

13) Any work performed to develop a preliminary output using software

in scoping and bounding determination, feasibility studies, prototype methodology development, or similar activities, as allowed by OSTI-LLNL-QIP-SI.0, is adequately documented. A checker comment shall be made documenting that additional checking is required when the work producing the final output is documented in the scientific analysis report. The check of the work producing the final output may be performed following the review for OSTI-LLNL-QIP-6.1, *Document Review*.

B. Clearly and legibly write, or mark electronically, all comments on the Checker Check Copy or indicate that there are no comments. (Comments may be documented separately if keyed to the Check Copy, and if comment documentation is signed, dated, and attached to the Check Copy.)

C. Initial and date the Checker Check Copy of Attachment 2.

D. Return documentation to the Originator.

3.3.4 QAR:

A. For scientific analyses subject to QAP requirements, perform a quality assurance (QA) compliance check to ensure compliance with this procedure and the applicable TWP. (Details of the compliance check may be documented on the QE Checklist in accordance with BSC LP-2.8Q-BSC, *Quality Engineering Checklists.)*

B. Clearly and legibly write, or mark electronically, all comments on the QAR Check Copy or indicate that there are no comments. Initial and date each comment. (Comments may be documented separately if keyed to the Check Copy and if comment documentation is signed, dated, and attached to the Check Copy.)

C. Initial and date the QAR Check Copy of the Scientific Analysis Signature Page/Change History and return the documentation to the Originator.

3.3.5 Originator:

A. Resolve all comments with the Checker and QAR and document resolution by mark up of the applicable Check Copy, including the proposed resolution for accepted comments and the rationale for any comments not incorporated or only partially incorporated. Initial and date each resolution. Use additional pages as necessary. Resolutions may be documented separately if keyed to the applicable Check Copy and the resolution documentation is signed, dated, and attached to the Check Copy.

B. Elevate unresolved comments to the next levels of management of the Originator and Checker/QAR until resolution is achieved and document the resolution. (Resolutions may be documented separately if keyed to the

applicable Check Copy.)

C. Modify the original scientific analysis documentation as required to incorporate comment resolution.

D. Denote the modified scientific analysis documentation (back check copy) by revising the alphanumeric revision designator.

E. Provide the back check copy, the DIRS report (when applicable), and the applicable Check Copy to the Checker and QAR.

3.3.6 Checker and QAR:

A. Check the modified scientific analysis documentation by comparing it to the applicable Check Copy.

B. Indicate acceptance of the resolution of each comment, including any comment that was not incorporated or was only partially incorporated by accepting the Originator's rationale or by providing separate justification. Initial and date each acceptance. Use additional pages as necessary.

C. Sign and date the applicable Check Copy of the Scientific Analysis Signature Page/Change History and return the documentation to the Originator.

3.3.7 Originator:

Prepare a review copy of the scientific analysis documentation and forward to the PI or Lead.

3.3.8 PI or Lead:

A. Initiate a review in accordance with OSTI-LLNL-QIP-6.1, as applicable (see Subsection 3.6 for review criteria related to changes).

B. Include organizations/disciplines providing input to the scientific analysis documentation, customer organizations/disciplines for the scientific analysis documentation, and organizations/disciplines affected by the scientific analysis documentation as mandatory reviewers on OSTI-LLNL-QIP-6.1 reviews of scientific analysis documentation.

C. Note any software products that must be baselined before the scientific analysis report can be approved or any data submitted to TDMS is finalized.

3.3.9 Reviewing Organization:

A. Complete a review of the scientific analysis documentation in accordance

with OSTI-LLNL-QIP-6.1.

B. If the scientific analysis does not affect or impact the Reviewing Organization, indicate "not applicable" and return the review documentation.

3.3.10 Originator:

A. Resolve all comments with the reviewers in accordance with OSTI-LLNL-QIP-6.1. Elevate unresolved comments to the next levels of management of the Originator and reviewers until resolution is achieved and document the resolution.

B. Develop a concurrence draft by modifying the OSTI-LLNL-QIP-6.1 review copy of the scientific analysis documentation, as required, to incorporate changes resulting from the comment resolution.

C. After the OSTI-LLNL-QIP-6.1 comments have been incorporated, provide the final concurrence copy of the scientific analysis documentation to the PI/Lead, Checker, and QAR.

3.3.11 PI/Lead, Checker, and QAR:

A. Ensure that the OSTI-LLNL-QIP-6.1 review comments, as resolved, have not adversely affected the scientific analysis documentation.

B. Resolve any adverse impacts with the Originator and the Reviewing Organization.

C. Indicate acceptance by signing and dating the Scientific Analysis Signature Page/Change History of the concurrence draft. Return the documentation to the Originator.

D. The QAR may document details of the compliance check on the QE Checklist in accordance with BSC LP-2.8Q-BSC.

E. If additional checking is required when the work producing the final output is documented in the analysis report, the Checker must complete that additional checking of the final output prior to the approval of the analysis report.

3.3.12 Originator:

If applicable, request lockout of changes to links in DIRS in accordance with BSC LP-3.15Q-BSC.

3.4 PRODUCT OUTPUT

It is not necessary for the action steps to be performed sequentially.

3.4.1 Originator:

A. Submit the following items to the TDMS in accordance with OSTI-LLNL-QIP-SIII.3:

1) Product output that replaces or supersedes product output or data that are currently in the TDMS.

2) Data that have undergone a status change, as a result of a qualification within the scientific analysis.

3) Other output may be submitted, as directed by the PI or Lead.

B. Finalize or supersede preliminary product output, if any, in accordance with OSTI-LLNL-QIP-SIII.3.

3.5 APPROVALS

3.5.1 Originator:

A. Prepare the scientific analysis documentation by changing the alphanumeric designator to a numeric designator (i.e., the initial technical product designator is "00," and subsequent revisions are "01," etc.) and update the change history as needed.

B. Complete the Scientific Analysis Signature Page/Change History in accordance with the instructions in Attachment 3.

C. Process the approved scientific analysis in accordance with OSTI-LLNL-QIP-6.0.

D. Submit supporting scientific analysis documentation to the Records Center in accordance with Section 6.0 of this procedure.

3.5.2 PI/Lead:

a) If modifications are required as a result of the OCRWM/OSTI review ensure the development and change process defined by this procedure is followed.

b) When applicable, if the document resolves DIRs TBVs/Unresolved Reference Numbers, process in accordance with BSC LP-3.15Q-BSC.

c) For any cases where the final output is not identical to the preliminary output, evaluate the impact and determine the extent of any necessary rework.

3.6 CHANGE CONTROL

3.6.1 PI/Lead:

A. When initiating a change to an existing document, notify Document Control of the impending action to ensure version control.

B. When a scientific analysis is changed, the entire product must be brought into compliance with current versions of relevant procedures.

C. Changes (revisions) to completed scientific analysis documentation shall be reviewed, and approved in the same manner as the original scientific documentation with the following specific exceptions:

1) Editorial corrections to scientific analysis documentation do not require check or review but shall be distributed as a revision to the scientific analysis documentation.

2) Changes associated with incorporation of outstanding approved Errata Sheets, removal of TBV numbers (with no other text content changes), or updating DIRS input status that have no impact on other scientific analyses or organizations do not require OSTI-LLNL-QIP-6.1 review.

3) Changes (e.g., additions or updates to appendices, addition of DTNs or other inputs, or additional assumptions) that have no impact on other scientific analyses or organizations do not require OSTI-LLNL-QIP-6.1 review.

D. Reviews and checks are limited to the procedurally required changes, actual changes, and the portions of the documentation affected by the changes.

E. Indicate changes in the scientific analysis documentation using one of the following:

1) A black vertical line in the margin of the page clearly indicating which individual sections or subsections were revised and a brief description change of the revision or change in Block 13 of Attachment 2.

2) A note in Block 11 of Attachment 2 indicating the entire documentation was revised because the changes were too extensive to use Step 3.6.E.1).

F. If desired and if the entire scientific analysis documentation is not being revised, use alphanumeric page designators (e.g., 10a) to avoid repaginating caused by the addition of text. If alphanumeric pagination is used, identify the alphanumeric page numbers inserted in the change history for future accountability. For clarity, alphanumeric pagination

should revert back to sequential page numbers in the next complete revision.

G. Maintain the history of all previous changes to the original on Attachment 2 by updating the Change History blocks with each revision.

H. Address any applicable errata, documented in accordance with OSTI-LLNL-QIP-16.0, in the appropriate section of the scientific analysis document. List any errata addressed in the Remarks section of the Scientific Analysis Signature Page/Change History.

I. Notify Document Control and, when applicable, DIRS/Reference Control of intention to cancel scientific analyses that are no longer relevant to the project. Obtain electronic mail acknowledgement from users prior to cancellation in accordance with OSTI-LLNL-QIP-6.0.

3.7 EDITORIAL CORRECTIONS

3.7.1 Originator:

A. If required to make editorial corrections to a document after approval, but prior to release for controlled distribution:

1) Make the correction(s) by drawing a single line through any incorrect text (i.e., pen/ink or electronic) and/or inserting any new or correct information.

2) Initial and date the correction(s).

3) Note the correction(s) in the Remarks section (Block 11) of Attachment 2.

B. Obtain the PI/Lead's approval of the change(s) adjacent to the notation on Attachment 2.

3.7.2 PI/Lead:

Initial and date Attachment 2 in the Remarks section, adjacent to the notation, to indicate approval of the correction(s).

4. RECORDS

The records listed in Section in 4.1 shall be collected and maintained in accordance with OSTI-LLNL-QIP-17.0, as individual records or included in a records package.

4.1 QA RECORDS

Records Package for Scientific Analysis subject to the QAP:

Checker and QAR Check Copies of the scientific analysis documentation

Comment Sheets or mark-ups containing comments

OSTI-LLNL-QIP-6.1 Review draft copy

Document Review Records, including attached criteria, if applicable

Final concurrence copy of OSTI-LLNL-QIP-6.1 review draft signed and dated on Scientific Analysis Signature Page/Change History by PI/Lead, Checker, and QAR

Records Submitted by Document Control per OSTI-LLNL-QIP-6.0:

Approved scientific analysis report

4.2 NON-QA LONG-TERM RECORDS

Records Package for Scientific Analysis not subject to the QAP:

Checker and QAR Check Copies of the scientific analysis documentation

Comment Sheets or mark-ups containing comments

OSTI-LLNL-QIP-6.1 Review draft copy

Document Review Records, including attached criteria, if applicable

Final concurrence copy of OSTI-LLNL-QIP-6.1 review draft signed and dated on Scientific Analysis Signature Page/Change History by PI/Lead, Checker, and QAR

Final copy of the DIRS report, when applicable.

Records Submitted by Document Control per OSTI-LLNL-QIP-6.0:

Approved scientific analysis report

4.3 NON-QA SHORT-TERM RECORDS (THREE YEARS OR LESS RETENTION)

Scientific Analyses Checklist(s), if completed by Originator and/or Checker

5. RESPONSIBILITIES

5.1 The **Project Manager** is responsible for, or designating a PI or Lead for, controlling the development, documentation, checking, change, and key technical activities of the scientific analysis activities in accordance with the requirements of this procedure.

5.2 The **QA Manager** is responsible for, or designating a Quality Assurance Representative for, conducting quality assurance compliance check of scientific analysis activities to ensure compliance with this procedure and applicable TWP.

5.3 **Staff Members** (PIs, Leads, Originators, Checkers, Reviewers, QARs, etc.) are responsible for the development, documentation, checking, change, and performance of the key technical activities of the scientific analysis activities in accordance with the requirements of this procedure.

5.4 The **Records Coordinator** is responsible for collecting and maintaining records associated with the development, documentation, checking, change, and performance of the key technical activities of the scientific analysis activities in accordance with the requirements of this procedure.

6. ACRONYMS AND DEFINITIONS

6.1 Acronyms

BSC	Bechtel SAIC Company, LLC
DI	Document identifier
DIRS	Document Input Reference System
DOE	U.S. Department of Energy
DTN	Data Tracking Number
EED	Energy & Environment Directorate
LLNL	Lawrence Livermore National Laboratory
M&TE	Measuring and Test Equipment
OCRWM	Office of Civilian Radioactive Waste Management
OQA	Office of Quality Assurance
OSTI	Office of Science & Technology and International
PI	Principal Investigator
PM	Project Manager
QA	Quality Assurance
QAP	Quality Assurance Program
QAR	Quality Assurance Representative
QARD	Quality Assurance Requirements and Description
QE	Quality Engineering
QIP	Quality Implementing Procedure
TAL	Technical Area Leader
TBV	To Be Verified
TDMS	Technical Data Management System
TWP	Technical Work Plan
YMRSP	Yucca Mountain & Repository Science Program

6.2 Definitions

Abstraction—The process of purposely simplifying a mathematical model

(component, barrier, or subsystem process model) for incorporation into an overall system model of the geologic repository. The products of model abstractions may represent reduction in dimensionality, elimination of time dependence, tables obtained from more complex models, response surfaces derived from the use of more complex models, representations of a continuous process or entity with a few discrete elements, etc.

Assumption—A statement or proposition that is taken to be true or representative in the absence of direct confirming data or evidence.

Checker—A qualified individual other than the Originator, technically competent in the subject area of the document undergoing checking, responsible for confirming adequacy, accuracy, and completeness of the scientific analysis documentation.

Editorial Corrections—Modifications made to a document, such as correcting grammar, spelling, or typographical errors; renumbering sections or attachments; and updating organizational titles. Editorial corrections do not affect the chronological sequence of work or the fundamental process, or alter assigned responsibilities.

Lead—An individual assigned by the Principal Investigator (PI) to control a scientific analysis activity and having responsibility for assignment of personnel to the scientific analysis activity.

Model, Mathematical—A mathematical representation of a conceptual model (system, process, or phenomenon) that is based on established scientific and engineering principles and from which the approximate behavior of a system, process, or phenomenon can be calculated within determinable limits of uncertainty.

Originator—A technically competent individual assigned responsibility for performing a scientific analysis, for preparing scientific analysis documentation (e.g., analyst, investigator, preparer), and for ensuring the adequacy, accuracy, and completeness of the scientific analyses documentation.

Principal Investigator—The individual having management responsibility for a scientific analysis activity, for assignment of a Lead to the scientific analysis activity, and for approving the scientific analysis documentation.

Scientific Analysis—A documented study that 1) defines, calculates, or investigates scientific phenomena or parameters; 2) evaluates performance of components or aspects of the overall geologic repository; or 3) solves a mathematical problem by formula, algorithm, or other numerical method. A scientific analysis may involve numerical manipulations that are not part of a previously developed and validated mathematical model (per QP-SIII.4Q, Models) if the choice of method is evident from standard scientific practice, approach, or method. A scientific analysis may also use a previously developed and validated mathematical model (per QP-SIII.4Q) consistent with the mathematical model's intended use and stated limitations, but may not revise the mathematical model in order to complete the scientific analysis.

Sensitivity—The degree to which the scientific analysis results are affected by

changes in a selected input.

To-Be-Verified (TBV)—Identification of information that is preliminary, needs to be reevaluated, and/or needs confirmation.

Traceability—The ability to trace the history, application, or location of an item, data, or sample using recorded documentation.

Transparency—The attribute of producing documents that are sufficiently detailed as to purpose, method, assumptions, inputs, conclusions, references, and units, such that a person technically qualified in the subject can understand the documents and ensure their adequacy without recourse to the Originator.

7. REFERENCES

DOE/RW-0333P, *Quality Assurance Requirements and Description*

BSC LP-3.15Q-BSC, *Managing Technical Product Inputs*

BSC LP-2.8Q-BSC, *Quality Engineering Checklists*

OSTI-LLNL-QIP-2.2, *Planning for Science Activities*

OSTI-LLNL-QIP-5.0, *Preparing the Quality Assurance Plan and Quality/Technical Implementing Procedures*

OSTI-LLNL-QIP-6.0, *Controlled Documents*

OSTI-LLNL-QIP-6.1, *Document Review*

OSTI-LLNL-QIP-16.0, *Condition Reporting and Resolution*

OSTI-LLNL-QIP-17.0, *Records Management*

OSTI-LLNL-QIP-SI.0, *Software Management*

OSTI-LLNL-QIP-SIII.0, *Scientific Notebooks*

OSTI-LLNL-QIP-SIII.3, *Submittal and Incorporation of Data to the Technical Data Management System*

OSTI-LLNL-QIP-SIII.4, *Qualification of Unqualified Data*

8. ATTACHMENTS

Attachment 1 – Scientific Analysis Outline

Attachment 2 – Scientific Analysis Signature Page/Change History

9. REVISION HISTORY

2/25/05 Revision 0, Modification 0
Initial issue.

10. APPROVALS

Preparer: Leigh Gouveia — Date: 2/25/05

Technical Reviewer: QINHONG HU — Date: 2/25/05

QA Reviewer: VICTOR J. BRADISH JR — Date: 2/25/05

Project Manager: DAVID B McCALLEN — Date: 2/25/05

SCIENTIFIC ANALYSIS OUTLINE

If any of the following sections are not applicable to a particular scientific analysis, a brief statement of non-applicability is required for documentation purposes under each heading. Information presented in the scientific analysis documentation shall be transparent and traceable.

1. **Purpose**—This section shall provide a statement of the purpose of the scientific analysis, the scientific analysis limitations, and the scope of the scientific analysis documentation. It shall also refer to the TWP for the activity and discuss, as necessary, any deviations from that plan.

2. **Quality Assurance**-This section shall include the applicability of the QA program, including evaluation of associated activities in accordance with appropriate implementing procedures. If scientific analyses or tasks included in the scientific analysis activity have been determined not to be subject to the QARD, provide justification. Reference the TWP for the determination of the applicability of the *QARD*. If the analysis investigates an item or barrier on the Q-List, identify the item or barrier and its safety category as classified in accordance with the applicable implementing procedure (AP-2.22Q, *Classification Analyses and Maintenance of the Q-List).* This section shall identify the method(s) used to control the electronic management of data in accordance with the controls specified in the TWP and will describe any variance from the planned method(s).

3. **Use of Software**—This section shall include a list of all controlled and baselined software as described in OSTI-LLNL-QIP-SI.0. Document the use of the software, including the software name, tracking number, version, operating environment (including platform and operating system), and range of use. Discuss why the software was selected and describe any limitations on outputs due to the selected software. Document that the use of the software was consistent with the intended use and within the documented validation range of the software.

   Include a list of any software that was used prior to qualification to develop a preliminary output.

   If the solution to the calculation or analysis package used to support this technical product is obtained using the standard functions of a commercial off-the-shelf software program (e.g., EXCEL, MATHCAD, or EARTHVISION) and the results are not dependent on the software program used, this software does not need to follow OSTI-LLNL-QIP-SI.0. If the results are not dependent on the software program, the actions performed (as indicated below) shall be documented in sufficient detail in this technical product to allow an independent reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the Originator:

   - The formula or algorithm used
   - A listing of the inputs to the formula or algorithm
   - A listing of the outputs from the formula or algorithm
   - Other information (e.g., operating environment information) that would be required in order for any independent person to reproduce the work.

4. **Inputs**—Project data shall be referenced by DTN. Technical product inputs shall be correctly selected, identified in the scientific analysis documentation, correctly cited, and incorporated.

4.1 **Direct Inputs**—The appropriateness of technical product inputs directly used to develop the scientific analysis shall be documented and substantiated in this section.

- Provide lists or tables of technical product inputs.
- If the present study uses a previously developed and validated model to complete the present study, list associated DTNs, accession numbers, documentation titles, and document identifying numbers, as applicable.

4.2 **Criteria**—List criteria identified in Section 3 of the TWP, including requirements contained in applicable requirement documents (such as design interface documents) and any relevant acceptance or completion criteria.

4.3 **Codes and Standards**—Provide a list of the applicable codes and standards used in the scientific analysis by name, number, and date, including applicable revision status, using date or revision designator.

5. **Assumptions**—This section shall include a description of the assumptions used, in the absence of direct confirming data or evidence, to perform the scientific analysis. Other scientific analysis assumptions are described in Section 6 of the analysis report.

6. **Scientific Analysis Discussion**—Describe the technical bases, mathematical formulations, and numerical methods used.

Provide (separate) lists or tables of corroborating/supporting data, models, product output, or technical information used in the scientific analysis activity. Identify the sources of the corroborating/supporting information. Document the qualification of unqualified project data developed in accordance with OSTI-LLNL-QIP-SIII.4. Include additional discussions to substantiate input used in this section, if not included in Section 4. Address any differences in direct input values, between values brought forward in Section 4, and values used in this section.

The following topics shall be included in this section, as applicable, when documenting a scientific analysis:

- A detailed description of the scientific approach and/or technical methods
- Results of literature searches or other background data/information
- A discussion of uncertainties, sources of uncertainties, and impacts of uncertainties on scientific analysis output
- Units of measurement
- A discussion of assumptions, idealizations, and simplifications, including their bases or rationale
- A discussion of scientific analysis assumptions (other than those made in the absence of direct confirming data or evidence), mathematical formulations, equations, algorithms, and numerical methods used

- Alternate scientific approaches and/or technical methods that were not used and the rationale for not selecting them
- Intended use of the output
- Comparison between the preliminary and final outputs, as applicable
- Appropriateness of the use of a previously developed and validated model to complete the present scientific analysis is described
- Other software/computational methods considered and the rationale for not selecting them.

7. **Conclusions**—This section shall provide a summary of the scientific analysis. The conclusions, including product output, as well as any decisions or recommendations, shall be presented in this section. Conclusions shall include any uncertainties and restrictions for subsequent use.

8. **Inputs and References**—Sources of inputs, software, DTNs, and cited references (including references used to justify assumptions) shall be listed in this section. Inputs and references include materials that support the conclusions of the scientific analysis. These may include published reports, technical papers, scientific notebooks, literature searches, or other background information. The OCRWM Style Manual (located on the BSC Intranet) may be used as guidance on formatting reference lists and citations.

Appendices—Supporting documentation, such as computer output, that are lengthy or cannot be conveniently included within the main text of the documentation may be included as appendices. Computer output may be attached as hard copy, read-only disk, or compact disk (read only memory), but must meet the requirements of OSTI-LLNL-QIP-17.0 for submittal to the TDMS. Computer output files included as appendices are exempt from page numbering, DI, and revision number requirements provided the total number of pages in each appendix (for hard copy) or complete file information including all file names, file dates and times, and file sizes are documented on the appendix. In case of printed appendices, the total page count for each appendix shall be documented on the Scientific Analysis Signature Page/Change History. Where the appendix is on computer media, the quantity and type of media shall be clearly identified on the Scientific Analysis Signature Page/Change History.

OSTI-LLNL	*Scientific Analysis Signature Page/ Change History*	Page iii
		1. Total Pages:

2. Scientific Analysis Title	
3. DI (including Revision Number)	
4. Total Appendices	5. Number of Pages in Each Appendix

	Printed Name	Signature	Date
6. Originator			
7. Checker			
8. QAR			
9. Responsible Manager/Lead			
10. Responsible Manager			

11. Remarks

Change History

12. Revision No.	13. Description of Change

INSTRUCTIONS FOR COMPLETING THE SCIENTIFIC ANALYSIS SIGNATURE PAGE/CHANGE HISTORY

Block Number

Originator

1. Enter the total number of pages (including appendices).

2. Enter the title of the scientific analysis.

3. Enter the DI, including the revision number, assigned to the scientific analysis.

4. Indicate total number of appendices.

5. Indicate the number of pages in each appendix (e.g., A-II, B-5, and c-20) or if list is long, identify where a listing is provided.

6. Print name, sign, and date.

Checker

7. Print name, sign, and date.

QAR

8. Print name, sign, and date when all comments have been resolved and changes have been incorporated into the scientific analysis.

PI/Lead

9. Print name, sign, and date to signify approval. (If a Lead was not assigned, the PI should complete this block.)

PI

10. Print name, sign, and date to signify approval,

Originator, Checker, QAR, Lead

11. Enter any pertinent remarks.

Originator

12. Identify any revisions to this scientific analysis, in order, starting with REV 00 and continuing to the latest revision.

13. For any revisions to this scientific analysis, enter a brief description of each change and the reason for the change (e.g., "added Appendices A and B"). If alphanumeric pagination is used, identify the alphanumeric page numbers inserted in the change history for future accountability.